Highlights of research results using the acquired NSF-MRI computers (Rutgers-Camden)

I.) Development of novel methodology: Structural determining under finite electric fields in density functional theory is a long-standing problem. We solved this problem by developing an efficient approach.

H. Fu and L. Bellaiche, Physical Review Letters 91, 057601 (2003).

II.) Exploring new research field: Nano-ferroelectrics

One critical problem in nanoferroelectrics is whether there exists ferroelectric instability in nano-dots. Our theoretical modeling say "yes" to this fundamental question. (see Fig.1)

Fu and Bellaiche, Fundamental Physics of Ferroelectrics, (2003)

Phys. Rev. Lett. (submitted).

III.) Studying new semiconductor nanostructures:
The wavefunction of the top-valence state of silicon quantum ring (Fig.2)

A. Nazzal and H. Fu, (unpublished)

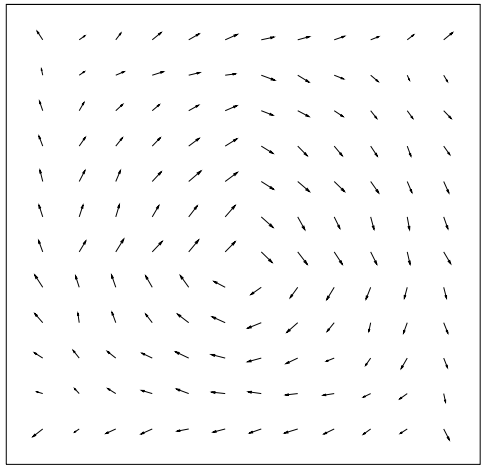

Fig.1

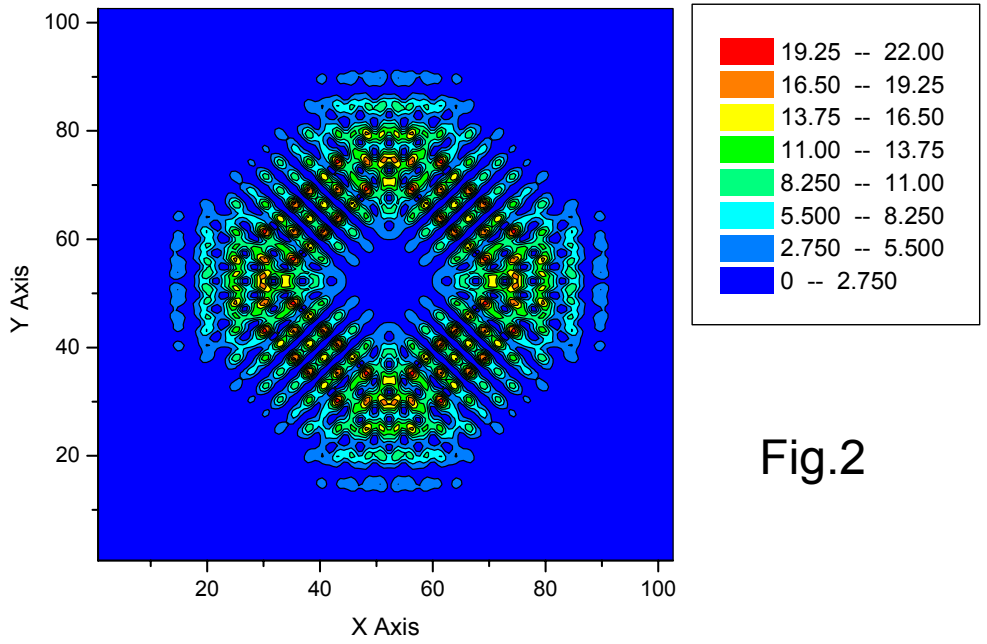

Fig.2